Complete Parameters for ReaxFF Reactive Force Field for C/H/Ni

Supporting Information for "Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel."
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This document contains the ReaxFF parameters in tabular form used for the Ni/C/H potential described above. Parameters in bold/italics were trained against the C/H/Ni training set presented in the above publication.

General Parameters

parameter	unit	value
$p_{boc,1}$	-	50.0000
$p_{boc,2}$	-	9.5469
$p_{coa,2}$	-	26.5405
$p_{trip,4}$	-	1.7224
$p_{trip,3}$	-	6.8702
kc_2	kcal/mol	60.4850
$p_{ovun,6}$	-	1.0588
$p_{trip,2}$	-	4.6000
$p_{ovun,7}$	-	12.1176
$p_{ovun,8}$	-	13.3056
$p_{trip,1}$	kcal/mol	-70.5044
$p_{val,7}$	-	33.8667
$p_{lp,1}$	-	6.0891
$p_{val,9}$	-	1.0563
$p_{val,10}$	-	2.0384

parameter	unit	value
$p_{pen,2}$	-	6.9290
$p_{pen,3}$	-	0.3842
$p_{pen,4}$	-	2.9294
$p_{tor,2}$	-	5.7796
$p_{tor,3}$	-	10.0000
$p_{tor,4}$	-	1.9487
$p_{cot,2}$	-	2.1645
$p_{vdW,1}$	-	1.5591
$B.O.\,Cutoff$	-	0.0010
$p_{coa,4}$	-	2.1365
$p_{ovun,4}$	-	0.6991
$p_{ovun,3}$	-	50.0000
$p_{val,8}$	-	1.8512
$p_{coa,3}$	-	2.6962

Atom Parameters

	r_o^{σ}	Val_i	m	r_{vdW}	D_{ij},	γ	r_o^{π}	Val_i^e	α	γ_w	Val_i^{angle}	p_{ovun5}	χ
	Å	-	amu	Å	kcal/mol	Å^{-1}	Å	-	-	Å^{-1}	-	kcal/mol	eV
C	1.3831	4.0000	12.0000	1.8814	0.1923	0.9000	1.1363	4.0000	9.7821	2.1317	4.0000	30.0000	5.9666
H	0.8873	1.0000	1.0080	1.5420	0.0598	0.6883	-0.1000	1.0000	8.1910	30.9706	1.0000	0.0000	3.5768
Ni	1.8201	2.0000	58.6900	1.9449	0.1880	0.8218	0.1000	2.0000	12.1594	3.8387	2.0000	0.0000	4.8038

	η	$r_o^{\pi\pi}$	p_{lp2},	I	p_{boc4}	p_{boc3}	p_{boc5}	p_{ovun2}	p_{val3}	Val_i^{boc}	p_{val5}
	eV	Å	kcal/mol	kcal/mol	-	-	-	-	-	-	-
C	7.0000	1.2071	0.0000	186.1720	9.0068	34.9357	13.5366	-2.8983	2.5675	4.0000	2.9663
H	10.5896	-0.1000	0.0000	54.0596	1.3986	2.1457	0.0003	-15.7683	2.1488	1.0000	2.8793
Ni	7.3852	-1.0000	0.0000	95.6300	50.6786	0.6762	0.0981	-3.7733	3.6035	2.0000	2.5791

Bond Parameters

	D_e^{σ}	D_e^{π}	$D_e^{\pi\pi}$	$p_{be,1}$	$p_{bo,5}$	13*corr*	$p_{bo,6}$	$p_{ovun,1}$	$p_{be,2}$	$p_{bo,3}$	$p_{bo,4}$	$p_{bo,1}$	$p_{bo,2}$
	kcal/mol	kcal/mol	kcal/mol	-	-	-	-	-	-	-	-	-	-
C-C	143.3883	96.3926	76.4404	-0.7767	-0.4710	1.000	34.9900	0.5108	0.4271	-0.1116	9.0638	-0.0840	6.7452
C-H	181.9084	0.0000	0.0000	-0.4768	0.0000	1.000	6.0000	0.7499	12.8085	1.0000	0.0000	-0.0608	6.9928
H-H	168.2342	0.0000	0.0000	-0.2191	0.0000	1.000	6.0000	1.0062	6.1152	1.0000	0.0000	-0.0889	6.0000
C-Ni	***83.5810***	***9.0383***	0.0000	***0.2531***	-0.200	1.000	16.0000	***0.0529***	***1.4085***	***-0.1113***	***13.3900***	***-0.1436***	***4.5683***
H-Ni	***114.7566***	0.0000	0.0000	***-0.8939***	0.0000	1.000	6.0000	***0.1256***	***0.1054***	1.0000	0.0000	***-0.1196***	***5.0815***
Ni-Ni	91.2220	0.0000	0.0000	-0.2538	-0.2000	0.000	16.0000	0.2688	1.4651	-0.2000	15.0000	-0.1435	4.3908

Off Diagonal Terms

	D_{ij}	R_{vdW}	α	r_o^{σ}	r_o^{π}	$r_o^{\pi\pi}$
	kcal/mol	Å	-	Å	Å	Å
C-H	0.1188	1.4017	9.8545	1.1203	-1.0000	-1.0000
C-Ni	***0.0800***	***1.7085***	***10.0895***	***1.5504***	***1.4005***	-1.0000
H-Ni	***0.0366***	***1.7306***	***11.1019***	***1.2270***	-1.0000	-1.0000

Angle Terms

	Θ_o	$p_{val,1}$	$p_{val,2}$	$p_{coa,1}$	$p_{val,7}$	$p_{pen,1}$	$p_{val,4}$
	degrees	kcal/mol	-	kcal/mol	-	-	-
C-C-C	72.7917	38.5829	0.7209	0.0000	0.1409	17.4509	1.0670
C-C-H	72.1533	14.2108	6.2512	0.0000	0.0100	0.0000	1.1022
H-C-H	73.2608	24.9703	3.7807	0.0000	0.1335	0.0000	3.0461
C-H-H	0.0000	0.0000	6.0000	0.0000	0.0000	0.0000	1.0400
C-H-C	0.0000	7.5000	5.0000	0.0000	0.0000	0.0000	1.0400
H-H-H	0.0000	27.9213	5.8635	0.0000	0.0000	0.0000	1.0400
C-Ni-C	***62.5000***	***16.6806***	***0.7981***	0.0000	***0.9630***	0.0000	***1.0711***
C-C-Ni	***87.6241***	***12.6504***	***1.8145***	0.0000	***0.6154***	0.0000	***1.5298***
Ni-C-Ni	***100.0000***	***40.4895***	***1.6455***	0.0000	***0.0100***	0.0000	***1.7667***
C-Ni-Ni	***5.0994***	***3.1824***	***0.7016***	0.0000	***0.7465***	0.0000	***2.2665***
H-Ni-H	106.3969	30.0000	0.9614	0.0000	1.9664	0.0000	2.2693
H-H-Ni	0.0000	***26.3327***	***4.6867***	0.0000	0.8177	0.0000	***1.0404***
Ni-H-Ni	0.0000	***60.0000***	***1.8471***	0.0000	***0.6331***	0.0000	***1.8931***
H-Ni-Ni	***30.3748***	***1.0000***	***4.8528***	0.0000	***0.1019***	0.0000	***3.1660***
H-Ni-Ni	180.0000	***-27.2489***	***8.3752***	0.0000	0.8112	0.0000	***1.0004***
C-Ni-H	***97.5742***	***10.9373***	***2.5200***	0.0000	***1.8558***	0.0000	***1.0000***
C-H-Ni	0.0000	***0.2811***	***1.1741***	0.0000	***0.9136***	0.0000	***3.8138***
H-C-Ni	***84.0006***	***45.0000***	***0.6271***	0.0000	***3.0000***	0.0000	***1.0000***

Torsion Terms

	V_1	V_2	V_3	$p_{tor,1}$	$p_{\cot,1}$
	kcal/mol	kcal/mol	kcal/mol	-	kcal/mol
C-C-C-C	-0.5000	53.0886	-0.1335	-6.2875	-1.9524
C-C-C-H	-0.4614	29.0459	0.2551	-4.8555	-2.7007
H-C-C-H	-0.2833	31.2867	0.2965	-4.8828	-2.4652
X-C-H-X	0.0000	0.0000	0.0000	0.0000	0.0000
X-H-H-X	0.0000	0.0000	0.0000	0.0000	0.0000
X-C-C-X	0.0000	50.0000	0.3000	-4.0000	-2.0000
C-C-C-Ni	0.0000	5.0000	0.4000	-6.0000	0.0000
Ni-C-C-Ni	0.0000	***44.3024***	***0.4000***	***-4.0000***	0.0000
H-C-C-Ni	0.0000	***21.7038***	***0.0100***	***-4.0000***	0.0000
H-C-Ni-C	0.0000	***5.2500***	***0.0100***	***-6.0000***	0.0000
C-C-Ni-C	0.0000	5.1676	0.0100	-5.9539	0.0000
C-C-Ni-H	0.0000	5.1676	0.0100	-5.9539	0.0000